

Theory of Multi-Band Superconductivity in Iron Pnictides

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The precise nature of unconventional superconductivity in Iron Pnictides is presently a hotly debated issue. Here, using insights from normal state electronic structure *and* symmetry arguments, we show how an unconventional SC emerges from the bad metal “normal” state. Short-ranged, multi-band spin- and charge correlations generates *nodeless* SC in the *active* planar $d_{xz,yz}$ bands, and an inter-band *proximity* effect induces out-of-plane gap nodes in the *passive* $d_{3z^2-r^2}$ band. While very good quantitative agreement with various key observations in the SC state *and* reconciliation with NMR and penetration depth data in the same picture are particularly attractive features of our proposal, clinching evidence would be an experimental confirmation of *c*-axis nodes in future work.

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High Temperature Superconductivity (HTSC) in the recently discovered Iron pnictides (FePn) is the latest surprise among a host of others in *d*- and *f* band materials [1]. HTSC arises upon doping (x) a spin-density-wave (SDW) *metal*: with $x > x_c$, SDW order melts, giving way to a HTSC. In the “normal” phase, with no SDW/SC order for $T > T_{SDW/SC}(x)$, various probes reveal an incoherent metallic state, presumably not too far from a Mott insulator [2]. HTSC in FePn arises from an *incoherent* normal state, at least in the FeAs-based materials, where a quasi-linear-in- T resistivity is seen immediately above T_c : this implies a correlated normal state. Local density approximation plus dynamical mean-field (LDA+DMFT) calculations in the intermediate-to-strong correlation limit [3, 4] indeed find very good *quantitative* agreement with a range of basic physical properties of FePn, attesting to their sizably correlated nature.

If SC is an instability of this incoherent metal, one expects pronounced deviations from weak-coupling BCS-like theories in the SC state, as in the cuprates: this is indeed borne out in experiments. Specifically, (i) the pair coherence length, ξ_{ab} is short ($< 20 \text{ \AA}$), the upper critical field, H_{c2} is high [5], with small superfluid density, (ii) the NMR relaxation rate, $T_1^{-1}(T) \simeq T^3$ [6], and the penetration depth in the 1111-FePn, $\lambda(T) \simeq T^n$ with $n = 2 - 2.5$ [7], indicating unconventional SC (U-SC). However, the 122-FePn seem to show conventional *s*-wave-like behavior, though, even here, the situation is controversial [7]. Moreover, μ SR studies reveal Uemura scaling and T_c vs ϵ_F scaling characteristic of other, well-known, correlated SC [8]. (iii) Optical measurements [9] show a large-scale spectral weight transfer (SWT) across T_c over an energy scale $> O(1.0) \text{ eV}$, while ARPES data show a sharpening of the low energy quasiparticle kink [10] below T_c . Taken together, as they must be, (i)-(iii) imply a strong coupling SC arising from an *incoherent* non-FL metal. Given (ii), the existence of gap nodes is an open, controversial, issue [11]. In particular, (i)-(iii) resemble observations in cuprates [12], implying

an U-SC closer to the Bose condensed, rather than the BCS limit [10]. How can such a U-SC arise as an instability of an incoherent normal state [3, 4]? How may nodes appear in the gap function? Does SC pairing involve all, or a subset of the Fe-*d* orbitals? These issues are of great import for FePn, and call for a systematic resolution. Here, motivated by the above, we focus on the 1111-FePn, specifically on $\text{LaO}_{1-x}\text{FeAsF}_x$. Guided by group-theoretical analyses, and by the *renormalized* multi-band structure, we propose a specific, strong correlation based, *interband* pairing mechanism for U-SC as an instability of the incoherent metal found in earlier LDA+DMFT studies [3, 4].

LDA+DMFT studies for the 1111-FePn find an incoherent, pseudogapped “normal” state, implying *blocked* coherent one-electron propagation: only collective motion of the spin and charge fluid is possible [13]. This opens the door to coherent *two*-particle propagation, i.e., to two-particle instabilities, to relieve the finite entropy at lower T . At $x = 0$, the electron- and hole-like Fermi surface (FS) sheets are nearly nested in LDA calculations, and DMFT will not alter this fact, since the self-energies are *local*; this favors the $\mathbf{q} = (\pi, 0)$ SDW instability, also within LDA+DMFT [3] (in fact, no nesting is needed at strong coupling [2, 3]), in agreement with neutron data [3, 14]. Doping weakens the SDW and facilitates the U-SC instability.

Since coherent one-electron transfer between different orbitals is blocked in the incoherent metal, we propose, in analogy with the situation encountered in coupled Luttinger liquids (LL) [15], that small, residual, inter-site and inter-orbital interactions mediate two-particle instabilities in FePn at low T . In principle, various types of instabilities, competing with U-SC [16], may be generated, as studied more extensively for cuprates [17]. Here, we focus on the U-SC alone. We further *assume* that pair formation primarily involves the *active* $d_{xz,yz}$ orbitals, and show that, due to the inter-orbital coupling U' , an interband (IB) proximity effect will induce SC on all FS sheets, as in Sr_2RuO_4 [18].

Excluding spin-triplet pairing, the general interaction in the cooper channel is

$$H_{pair} = \frac{1}{2} \sum_{a,b,k,k'} V_{ab}(k,k') c_{a,k,\uparrow}^\dagger c_{b,-k,\downarrow}^\dagger c_{b,-k',\downarrow} c_{a,k',\uparrow},$$

where $a, b = xz, yz$ and the scattering vertex is $V_{ab}(k, k', \omega) = g^2 \chi_{ab}(k - k', \omega)$ with $\chi_{ab}(k - k', \omega)$ being the *inter*-orbital susceptibility. Such a term naturally arises at second order from a one-electron inter-band term, $t_{ab} \sum_{\langle i,j \rangle, \sigma} (c_{ia\sigma}^\dagger c_{jb\sigma} + h.c.)$, when the one-electron spectral function is incoherent, much like in coupled LL [19]. This is an important feature of our work: normal state one-particle incoherence, arising from the Anderson orthogonality catastrophe [3, 4] due to strong multi-orbital correlations, favors two-particle coherence. The *static*, nearest- and next-nearest neighbor parts of $V_{ab}(k, k')$ are $V_{ab}^{(1)}(k, k', 0) \simeq \frac{t_{ab}^2}{U' + J_H} \simeq O(40 - 50)$ meV and $V_{ab}^{(2)} \simeq \frac{t_{ab}^2}{U' + J_H} \simeq O(15 - 20)$ meV, close to the superexchange scale estimated from inelastic neutron scattering (INS) studies [20]. Notice that the effective interaction contains coupled inter-orbital charge and spin fluctuations involving nearest (n.n) and next-nearest neighbor (n.n.n) Fe sites, and is explicitly \mathbf{k} -dependent, favoring U-SC from the outset. H_{pair} can be decoupled *a la* Gorkov [21] to yield

$$H_{pair}^{MF} = \sum_{a,b,k} [\Delta_{ab}(k) c_{k,a,\uparrow}^\dagger c_{-k,b,\downarrow}^\dagger + h.c.],$$

where $\Delta_{ab}(k) = \frac{1}{2} V_{ab}(k) \langle c_{-k,b,\downarrow} c_{k,a,\uparrow} \rangle$ is the SC gap function. Consistent with lattice symmetry, and including the n.n and n.n.n contributions, $V_{ab}(k, k') = \sum_l V_{ab}^l \eta_l(k) \eta_l(k')$, where the $\eta_l(k)$ are irreducible representations of D_{4h} point group. So we can expand $\Delta_{ab}(k) = \sum_l \Delta_{ab}^l \eta_l(k)$ [21]. Explicitly, $\Delta_{ab}(k) = \Delta_1(c_x + c_y) + \Delta_2 c_x c_y$, with $c_\alpha = \cos k_\alpha$. The case $\Delta_2 = 0$ (B_{2g} representation of D_{4h}) is favored in the numerical study [22], however, $\Delta_2 \neq 0$ is rigorously *required* [23]. With well-separated electron- and hole-like FS sheets as in LDA, no in-plane nodes exist in the SC gap for Δ_2/Δ_1 in the chosen range. A $\Delta_2 \neq 0$ is also favored by the observation of appreciable geometric frustration in FePn, where $J_2/J_1 \simeq O(0.7 - 1.0)$ have been deduced from *ab-initio* studies, and consistent with INS results [20].

The “normal” state is modelled by a five-band Hubbard model, $H_n = H_0 + H_1$, treated earlier with LDA+DMFT [3, 4], and reads $H_0 = \sum_{k,\alpha} \epsilon_{k,\alpha} c_{k,\alpha,\sigma}^\dagger c_{k,\alpha,\sigma}$ while $H_1 = U \sum_{i,\alpha} n_{i,\alpha,\uparrow} n_{i,\alpha,\downarrow} + U' \sum_{i,\alpha \neq \beta} n_{i,\alpha} n_{i,\beta} - J_H \sum_{i,\alpha \neq \beta} \mathbf{S}_{i,\alpha} \cdot \mathbf{S}_{i,\beta}$, where $\alpha, \beta = xy, yz, zx, x^2 - y^2, 3z^2 - r^2$. In the U-SC phase, we have to solve $H = H_n + H_{pair}^{MF}$ within LDA+DMFT. Fortunately, the *intersite* nature of H_{pair} adds simply a term bilinear in fermions to H . The LDA+DMFT equations are now readily extendable to the U-SC regime:

the \mathbf{G}_{ab} and Σ_{ab} now have normal and anomalous components, and a closed set of DMFT equations, yielding both G_{aa}, F_{ab} selfconsistently, is solved by extending earlier LDA+DMFT [4] to include an explicit pair-field term. Including the pair-field, the propagators are $G_{aa}(k, \omega) = [\omega - \epsilon_{ka} - \Sigma_a(\omega) - \frac{\Delta_{ab}^2(k)}{\omega + \epsilon_{kb} + \Sigma_b^*(\omega)}]^{-1}$ and $F_{ab}(k, \omega) = G_{aa}(k, \omega) \frac{\Delta_{ab}(k)}{\omega + \epsilon_{kb} + \Sigma_b^*(\omega)}$, where the $*$ denotes complex conjugation. Given *intersite* pairing, $F_{ij,ab}(\omega)$ falls off at least as $\frac{1}{\sqrt{D}}$, (here, D is the lattice dimension) the *dynamical* effects of these non-local pair fluctuations do not enter the DMFT *self-energies*. Obviously, however, they do affect the G_{aa} s. Our treatment is thus different from that of Garg *et al.* [24], where the dynamical effects of *local* pair fluctuations must be kept in DMFT. Anomalous contributions like $\Sigma_{i,j,ab}^{(2)}(t) = -V_{ab}^2 G_{i,i,aa}(t) F_{i,j,ab}(-t) G_{j,j,bb}(t)$, etc, to the *dynamical* self-energy would thus enter in a cluster-DMFT approach, but drop out in $D = \infty$. It then suffices to use the DMFT with the modified matrix propagators above. Finally, since these equations couple *all* Fe-*d*-orbitals, the opening up of a SC gap in the $d_{xz,yz}$ bands could induce secondary gaps in the remaining *d* orbitals, in a way reminiscent of the inter-band proximity effect in Sr_2RuO_4 [18] (see below). Further, given sizable $U = 4.0$ eV, $U' = 2.6$ eV for FePn [3, 4], large spectral changes within DMFT-like approaches should accompany the U-SC instability: these are seen in spectral probes [8, 9]. Is such a scenario also consistent with other signatures of a strong coupling, U-SC?

Aiming to shine light on these issues, we now describe our results. Upon convergence of the DMFT equations, the one-electron- and pair spectral functions can be read off and used for direct comparison with observables in the U-SC state. In Fig 1, we show the changes induced by U-SC in the *total* one-electron DOS. Clear sharpening of the low-energy kink at $\Omega \simeq 20.0$ meV [10, 25], already somewhat visible in the “normal” state [26], is seen across the U-SC instability. Strong normal state incoherence ($\Sigma_b^*(\omega)$ in the equation for $G_{aa}(\mathbf{k}, \omega)$) prevents opening up of a clean SC gap in the DOS, as indeed observed in PES. Remarkably, the *position* of this kink and the detailed PES *lineshape* up to a binding energy of -0.5 eV are both quantitatively reproduced within our theory.

More microscopic insight is obtained by investigating the orbital resolved DOS. As seen from Fig 2, only the $d_{xz,yz}$ and $d_{3z^2-r^2}$ DOS show the sharpening of the kink feature. Moreover, dominant SWT occurs *from* the d_{xy} band to the $d_{xz,yz,3z^2-r^2}$ bands, as clearly seen in Fig. 2. The first implies an orbital *selective* coupling of the carrier propagators to multi-orbital, overdamped and short-ranged, charge- and spin correlations, and fully agrees with indications from ARPES studies [25], which show clear evidence thereof. Large SWT, over an energy scale $O(2.0)$ eV, also accompanies the U-SC instability. This is also in qualitative accord with findings in optical stud-

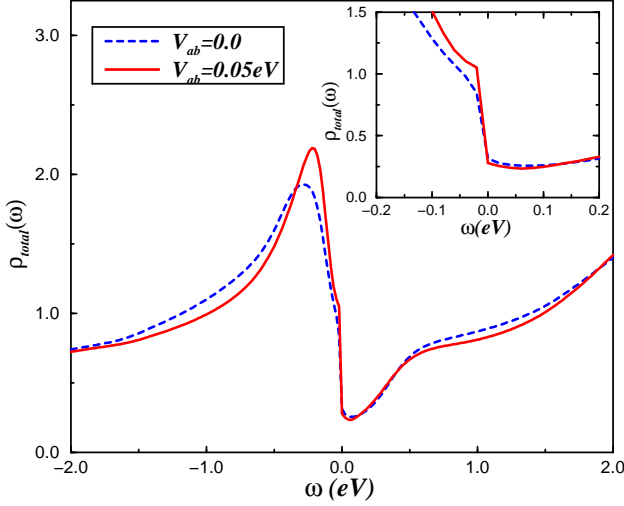


FIG. 1: (Color online): Evolution of the total one-particle density-of-states (DOS) across the superconducting transition for doped ($x = 0.1$) $LaO_{1-x}FeAsF_x$, for $U = 4.0$ eV, $U' = 2.6$ eV, and the effective interaction, $V_{ab} = \max(V_{ab}^{(1)}, V_{ab}^{(2)}) = 50$ meV. The inset shows how the low-energy kink, already visible above T_c (dashed curve), sharpens up below T_c (dotted curve), in very good agreement with ARPES data [10, 25].

ies [8]. Taken together, these findings imply a strong coupling SC, and fully accord with other observations in the SC state in FePn, as shown below.

Additional fundamental features of interest are gleaned from observation of the sharpening of the kink in the $d_{3z^2-r^2}$ DOS in the U-SC state above. This strongly suggests that an IB-proximity driven, out-of-plane SC gap component should enter on symmetry grounds. Examination of the Slater-Koster fit to the LDA shows a sizable $d_{xy} - d_{3z^2-r^2}$ mixing [27]; this will induce a $\Delta' \cos(k_z c)$ component, reduced by dipolar reduction factors [18], in the SC gap function. Strong supportive evidence for this comes from extant dHvA studies on $LaFePO$ [28]. This indeed shows *significant* warping of the d_{xy} band along the c -axis in the *non-magnetic* state, caused precisely by the mixing with the $d_{3z^2-r^2}$ pocket states. While correlation effects (LDA+DMFT) result in band shifts and dynamical SWT, they will leave the LDA FS unchanged, since the self-energies are purely *local*: this observation should hold for the 1111-FePn in general. Such interband one-particle mixing between the xy and $3z^2 - r^2$ bands induces an additional $\cos(k_z c)$ component in $\Delta_{ab}(\mathbf{k})$, giving possible line nodes in the SC gap function along k_z . This may be theoretically checked by closely following earlier analysis for another multi-band U-SC, Sr_2RuO_4 [18].

Generation of line nodes along c is *not* in conflict with extant ARPES results, as seen in $(Sr/Ba)_{1-x}K_xFe_2As_2$ [10]. Moreover, it can naturally explain the NMR and penetration depth data, being ca-

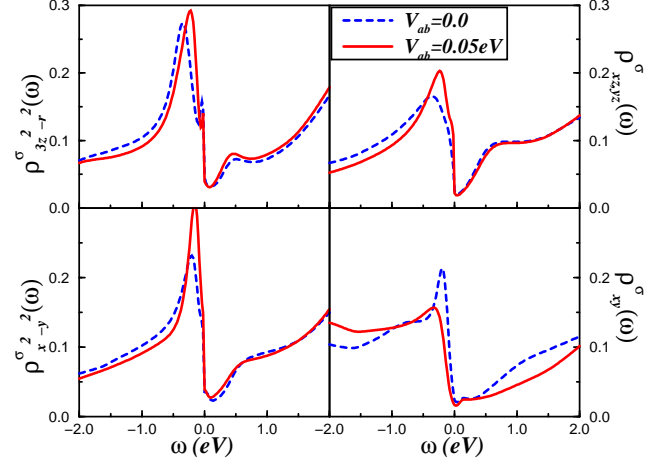


FIG. 2: (Color online): Orbital resolved evolution of the one-particle DOS across T_c , for the same parameter set as in Fig. 1. The orbital-selective gap structure, arising from multi-band correlations, is manifest. This is manifested in the orbital-selective sharpening of the low-energy kink, in qualitative accord with ARPES [10, 25].

pable of giving the observed power-law-in- T behavior for both the NMR $T_1^{-1}(T)$ [6] and $\lambda_{ab}(T)$ [7] at low $T \ll T_c$. In contrast to the s_{\pm} gap with disorder scenario [29], existence of nodes would imply *universal* power-law dependences in these quantities as a function of x , and along differing FePn members, as recently seen [7].

We emphasize that whether nodes along k_z exist or not is a delicate matter, and that a careful examination of the details of the band structure should provide invaluable clues. For example, dHvA study [28] on $LaFePO$ indeed finds sizable c -axis corrugation of the d_{xy} band, indicating sizable IB-proximity, and, interestingly, $\lambda_{ab}(T) \simeq T^{1.2}$ [28], strongly suggesting line nodes in the SC gap. However, data on $SmFeAsO_{1-x}F_x$ [32] are consistent with a *smooth* (nodeless) angular variation, $\Delta(\phi) = \Delta_0(1 + \epsilon \cos 4\phi)$, of the in-plane gap, and $\lambda_{ab}(T)$ follows the well-known $e^{-\Delta(\phi)/kT}$ law. In the FeAs materials, it is conceivable that the multiband coupling does *not* always induce out-of-plane nodes in the SC gap; this will be sensitive to the detailed topology of the *renormalized* FS. In cases where a non-exponential $\lambda(T)$ is seen, we suggest that dHvA results should show significant c -axis warping of the d_{xy} -FS sheet: this should be investigated in more detail. However, the planar $(1 + \epsilon \cos 4\phi)$ variation deduced for Sm-based FePn is not inconsistent with our in-plane form factor, as proposed above. Additionally, recently, INS work on Ni -doped $BaFe_2As_2$ clearly shows *both* planar and c -axis variation of $\Delta(\mathbf{k})$; interestingly, precisely $\Delta(k_z) \simeq \cos(k_z c)$ was found there [11]. It would be very interesting to see if this is also true

of the 1111-FePn. We then predict that this should be correlated with the c -axis warping of planar d_{xy} band in dHvA work. This would constitute a non-trivial check of our proposal.

From LDA+DMFT, we estimate the gap magnitude to be $\Delta_{ab} \simeq 4.5$ meV, close to that found in PES [33]. Using the carrier Fermi velocity from LDA (note that this is not changed by LDA+DMFT), $v_F \simeq 0.7$ eV.Å, the relation $\xi = v_F \hbar / \pi \Delta$ gives $\xi \simeq 60 - 80$ Å, close to observed values. The upper critical field is now estimable as $H_{c2} = \phi_0 / 2\pi \xi^2 \simeq 50 - 70$ T, (ϕ_0 is the usual flux quantum) again consistent with experiment [5]. These are classic signatures of a strong coupling SC [34], and require an instability of a strongly correlated *incoherent* “normal” state, as proposed here.

Our proposal is distinct from other, extant ones [11, 16, 20, 22, 30]. The s_{\pm} proposal [16, 30] is derived from a weak-coupling instability of an *itinerant* FL. Wu *et al.* [31] derive a similar state from the strong coupling limit of a reduced two-band model. The alternative, extended- s wave idea gives *eight* nodes on the electron-FS sheets [11, 20, 22]. Our proposal is a generalization of the s_{\pm} proposal [30, 31]. *All* earlier proposals, however, cannot access possible c -axis nodal structure, which arises via an IB proximity effect involving $d_{xy} - d_{3z^2-r^2}$ bands in our work. Moreover, rigorous analysis [23] and the geometrically frustrated superexchanges [2, 20] in FePn require *both*, Δ_1, Δ_2 to be finite. This naturally leads to k -dependent $\Delta_{ab}(k)$, as deduced experimentally [11, 32]. Finally, the U-SC derived here arises as an instability of the correlated, incoherent metal [3, 4] “normal” state seen in doped FePn, and naturally explains large spectral changes [9] and orbital selective sharpening of the QP kink [10] across T_c as manifestations of proximity to a Mott insulator [2, 3, 4].

In conclusion, we have derived the instability of the incoherent “normal” state of FePn [3, 4] to an U-SC. Blocking of inter-band one-particle *coherence* in the normal state clears the way for inter-band *two-particle* coherence to emerge, much like in coupled LLs, giving a multi-orbital SC with nodes. The latter are shown to arise from a multiband proximity effect between the d_{xy} and the $d_{3z^2-r^2}$ bands. Extending earlier LDA+DMFT calculations for the incoherent metal, we show how good *quantitative* agreement with the sharpening of the low-energy kink in the PES spectrum in the U-SC phase, as well as strong spectral weight transfer across the U-SC transition, is obtained. Further, induction of line nodes due to the interband proximity effect offers a reconciliation of these attractive features with NMR and μ SR data, which suggest existence of line nodes in the U-SC gap. Taken together, these strongly support our proposal of an U-SC with a planar $\Delta_{ab}(\mathbf{k}) \simeq (c_x + c_y) + \alpha c_x c_y$ form factor; i.e, a SC with co-existent, *inter-site* (and inter-orbital) s^* and s_{xy} pair symmetries, and out-of-plane nodes $[\Delta_c(\mathbf{k}) \simeq c_z]$, at least in some of the 1111-FePn

family. Our proposal calls for careful experimental search for the out-of-plane nodes in the 1111 Iron Pnictides.

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